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**Annual Report N00014-86-K-0736-P00003**

Period: Jan. 1, 1987 - April 1, 1988

Principal Investigators: S. Doniach
I. Lindau
Stanford Electronics Lab

A) <u>EXPERIMENTAL</u>: Studies of Schottky barrier formation at metal-semiconductor interfaces.

### (i) Initial stages of band bending

A systematic kinetics study of the initial stage of band bending of metal/GaAs(110) has been done.[1,2] At low temperature, independent of metals, enhanced band bending for p-GaAs and attenuated band bending for n-GaAs as a function of metal coverage has been observed. For p-type GaAs the band bending increases very rapidly to a value larger than that for any coverage at room temperature and then returns to the room temperature position at high coverages. It is found that this excess band bending strongly depends on the work functions of the metal deposited on GaAs. In gives 0.4eV, Al 0.3eV, Ag 0.2eV, and Au only shows small excess band bending. The results strongly suggest that there exists another mechanism which appears to be dominant in the initial stage band bending at low temperature where the defect formation is negligible.

The In growth on cleaved GaAs(110) surfaces at room temperature (RT) and 80 K low termperature (LT) as well as the initial stage Schottky barrier formation at this interface has been studied using photoelectron spectroscopy.[3] In grows as 3-D islands at RT, but in Stanski-Krastanov mode at LT. The size of the clusters has been estimated through an intensity study. The In core level spectra continuously shifts to high binding energy direction in the transformation from isolated atoms to bulk metal. The Fermi level pinning pattern shows a strong temperature dependence, which challenges current models of Schottky barrier formation at metal/semiconductor interfaces.

### (ii) Nature of the Sb/GaAs Interface

The temperature dependence of the development of the Sb/GaAs electronic properties has been found to be quite small, compared to that seen with a large number of metal/GaAs interfaces studied previously.[4,5] This has been correlated with the relatively small change in interface morphology due to reducing the temperature. The interface morphology

and the Fermi level movement at the Sb/GaAs(110) interface were studied using photoelectron spectroscopy (PES) at room temperature and low temperature (150 K and 80 K). The Sb/GaAs interface is uniform and abrupt at both temperatures. Two distinct Fermi level pinning positions are observed: 0.75eV for n-type GaAs and 0.5eV for p-type GaAs above the valence band maximum independent of the temperature.

(iii) Physical nature of near-surface defect acceptor and donor states on InP.[6,7]

The initial stage [0.001-30 monolayers (ML)] of room-temperature Schottky-barrier formation of In on n- and p-type InP(110) interfaces has been studied by photoemission using a newly designed ultralow-coverage metal evaporator which can reproducibly evaporate metals with coverages as low as 0.0001ML. It is found that the In/n-type InP(110) interface band bending does not start until the In coverage reaches about 0.3 ML, while the In/p-type InP(110) band bending is almost saturated at 0.3 ML. The heating effect on the band bending of clean cleaved n-and p-type InP(110) surfaces is also studied by using photoemission. It is found that heating has an irreversible band-bending effect on the p-type InP(110) but not on the n-type InP(110) interface. Based on these two striking differences in the band-bending behavior of n- and p-type InP, it is proposed that the physical nature of InP near-surface defect acceptor and donor levels may be different.

## B) THEORETICAL:

### 1. "High-$T_c$" Oxide Superconductors

The high critical temperatures measured in the copper oxide superconductors $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{7-y}$, and $CaBi_2Sr_2Cu_2O_8$ strongly suggest a pairing mechanism of electronic, rather than phononic, origin. In addition, proximity to metal-insulator and magnetic transitions as well as photoemission experiments, indicate the existence of large on-site Coulomb interactions. We have studied a number of models of the strongly interacting Cu-O planes in these materials using "slave boson" techniques to treat the local correlations. Preliminary results[8] indicated that large critical temperatures on the order of a fraction of J, the superexchange constant, were indeed possible. In this mean field analysis, superconductivity is caused by the virtual charge fluctuations which also give rise to antiferromagnetic order in the case of one electron per Cu site. We then investigated the possibility that such interactions could lead to coexistence of antiferromagnetism and superconductivity under certain circumstances.[9]

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This analysis, which indeed indicated coexistence but which clearly overestimated the stability of the ordered antiferromagentic state with respect to doping, led us to consider the effects of quantum fluctuations on the Neel order, as well as question whether a single-band correlated (Hubbard) model would be sufficient to describe the physics of the Cu-O system. The first investigation led to the construction of an effective spin representation of the Hubbard Hamiltonian in the case of less than one electron per site, and indeed showed a dramatically heightened sensitivity of the long range ordered Neel state to doping-induced disorder.[10,11] The second analysis led to a mean-field slave boson calculation for a 3-band copper oxide model. This has yielded a renormalized "quasiparticle" band structure for the Cu-O plane which in fact resembles the measured photoemission spectrum. Work along these lines, including calculations of the magnetic phase diagram and of optical spectra, is in progress.

2. Heavy Fermion Superconductors

While the origin of the microscopic pair interactions in the "heavy fermion" superconductors $UBe_{13}$, $Upt_3$, and $CeCu_2Si_2$ is still unclear, a simple phenomenological picture of the superconducting state which has been put forward in the past few years seems to be consistent with most thermodynamic and transport data. This invokes two hypotheses: 1) the existence of a highly anisotropic superconducting order parameter, with lines or points of nodes on the Fermi surface, and 2) the presence in virtually all samples of defects which act as Kondo or "resonant" scattering centers. We have continued a program of calculating various transport properties to confirm this picture and serve as a guide for a microscopic theory.[12] In this context we recently completed a calculation of the electromagnetic absorption[13] in such an anisotropic superconducting state, which shows frequency and temperature-dependent conductivities which differ dramatically from ordinary BCS superconductors. Such an experiment is the only way to observe in superconductors the collective order-parameter modes which should be characteristic of an unconventional superfluid, as in $^3He$. In addition, we have considered the question of how unconventional superconductivity could be detected in other ways. In a recent publication[14] it was shown that a cubic unconventional superconductor could exhibit a small but measurable magnetic response to an externally applied thermal gradient. This response would be rigorously zero in an isotropic system.

Publications


1. "Transition from Schottky limit to bardeen limit in the Schottky barrier formation of Al on n- and p-GaAs(110) interfaces," K.K. Chin, R. Cao, T. Kendelewicz, K. Miyano, M.D. Williams, S. Doniach, I. Lindau and W.E. Spicer," Mat. Res. Soc. Symp. Proc. 77, 297 (1987).

2. "Kinetics study of initial stage band bending at metal GaAs(110) interfaces," R. Cao, K. Miyano, T. Kendelewicz, K.K. Chin, Ingolf Lindau and W.E. Spicer." J. Vac. Sci. Technol. B 5 (4), 998 (1987).

3. "Growth mode and initial stage schottky barrier formation at the In/GaAs interface: a photoemission study," R. Cao, K. Miyano, K. Chin, I. Lindau, and W. E. Spicer, submitted for publication.

4. "Unusual low temperature behavior of fermi level movement at the Sb/GaAs Interface," R. Cao, K. Miyano, I. Lindau and W.E. Spicer, submitted for publication.

5. "Photoemission investigation of Sb/GaAs(110) interfaces," R. Cao, K. Miyano, T. Kendelewicz, I. Lindau and W.E. Spicer, submitted for publication.

6. "Photoemission study of the physical nature of the InP near-surface defect states," K.K. Chin, R. Cao, T. Kendelewicz, K. Miyano, J.J. Yeh, S. Doniach, I. Lindau, and W.E. Spicer," Mat. Res. Soc. Symp. Proc. 77, 429 (1987).

7. "Physical nature of the InP near-surface defect acceptor and donor states," K.K. Chin, R. Cao, T. Kendelewicz, K. Miyano, J.J.Yeh, I. Lindau, and W.E. Spicer, Phys. Rev. B 36, 5914(1987).

8. "Slave boson theory of superconductivity in a single-band Hubbard model,"A.E. Ruckenstein, P.J. Hirschfeld and J. Appel, Phys. Rev. 36, 857 (1987).

9. "Coexistence of magnetism and superconductivity in a mean field theory of the Hubbard model," M. Inui, P. Hirschfeld, S. Doniach and A.E. Ruckenstein, Phys. Rev. B, February, 1988.

10. "Quantum frustration and the disappearance of two-dimensional off-diagonal long range order at zero temperature," S. Doniach, M. Inui, V. Kalmeyer, and M. Gabay, submitted for publication.

11. "Doping dependence of antiferromagnetic correlation in high temperature superconductors," M. Inui, S. Doniach and M. Gabay, submitted for publication.

12. "Thermodynamic and transport properties of anisotropic superconductors," P. Hirschfeld, P. Wolfle and D. Einzel, Phys. Rev. B 37 (1988).

13 "Electromagnetic absorption in heavy fermion superconductors," P. Hirschfeld, P. Wolfle, J. Sauls and D. Einzel, submitted to Phys. Rev. B.

14. "Thermoelectric effect as a test of exotic superconductivity," P.J. Hirschfeld, to be published in Phys. Rev. B, June 1, 1988.